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Some current issues in quasi-Monte Carlo methods

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Abstract

We briefly discuss the following issues in quasi-Monte Carlo methods: error bounds and error reduction, optimization of net constructions, and randomization and derandomization.

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Quasi-Monte Carlo methods are deterministic versions of Monte Carlo methods. These methods have found many applications in scientific computing. See [3] for a recent survey on Monte Carlo and quasi-Monte Carlo methods. Detailed information on classical applications of quasi-Monte Carlo methods is available in [19,20]. New types of applications have recently been developed, in areas such as computational finance (see [34]), statistics (see [6]), stochastic differential equations (see [30]), and stochastic optimization (see [38]).

As befits a short note originating from a problem session, this is not a systematic survey, but rather a collection of quasi-random thoughts on some current issues in quasi-Monte Carlo methods. In the same vein, the bibliography is not comprehensive, but is meant to provide only some pointers to the literature. We address three topics which, from an admittedly subjective perspective, we find of particular interest at present: error bounds and error reduction, optimization of net constructions, and randomization and derandomization.

(i) *Error bounds and error reduction*. We consider the usual setting of quasi-Monte Carlo methods for numerical integration in which the integration domain is the

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s-dimensional unit cube $I^s := [0,1]^s$. We recall the classical Koksma–Hlawka bound

$$\left| \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{x}_n) - \int_{I^s} f(\mathbf{t})\, d\mathbf{t} \right| \leqslant V(f) D_N^*(\mathscr{P})$$

for any integrand f of bounded variation $V(f)$ on I^s in the sense of Hardy and Krause, where $D_N^*(\mathscr{P})$ is the star discrepancy of the node set $\mathscr{P} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset [0,1)^s$. Another classical result is Proinov's error bound $4\omega(f; D_N^*(\mathscr{P})^{1/s})$ for any continuous function f on I^s with modulus of continuity $\omega(f; \cdot)$. Both bounds have recently been generalized by Götz [9] who considered differences of integrals with respect to arbitrary Borel probability measures on I^s. Furthermore, many analogs of the Koksma–Hlawka bound have been found recently by Hickernell [10,11], who used a method based on reproducing kernel Hilbert spaces. This method has also been described in an abstract setting by Amstler and Zinterhof [2].

In a different direction, Niederreiter [21] established error bounds for node sets with special uniformity properties. Such node sets are often used in practice. Let λ_s be the s-dimensional Lebesgue measure and let $\mathscr{M}$ be a nonempty collection of Borel sets in I^s. Then a point set $\mathscr{P}$ of N points in I^s is called $(\mathscr{M}, \lambda_s)$-*uniform* if, for all $M \in \mathscr{M}$, the number of points of $\mathscr{P}$ falling into M is equal to $\lambda_s(M)N$. A typical result from [21] says that if $\mathscr{M}_r$ is the obvious partition of I^s into cubes of edge length $\frac{1}{r}$ and $\mathscr{P} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ is $(\mathscr{M}_r, \lambda_s)$-uniform with $N = r^s$, then

$$\left| \frac{1}{N} \sum_{n=1}^{N} f(\mathbf{x}_n) - \int_{I^s} f(\mathbf{t})\, d\mathbf{t} \right| \leqslant \omega(f; N^{-1/s})$$

for any bounded Lebesgue-integrable function f on I^s. This is considerably better than Proinov's bound. The methods of proof in [21] work in a quite abstract setting and lead to new types of problems in quasi-Monte Carlo integration, for instance, on the distance of functions (in a suitable function space) from linear subspaces spanned by characteristic functions.

Since all these error bounds are, in general, very pessimistic, one may take a cue from Monte Carlo methods and try to adapt variance reduction techniques to quasi-Monte Carlo methods to reduce the integration error. A variance reduction technique that can be applied in a straightforward manner to quasi-Monte Carlo methods is that of antithetic variates. This technique is basically the same as an old symmetrization trick in quasi-Monte Carlo methods; see [19, Section 4] as well as [1] for more recent work. Importance sampling is another variance reduction technique that can be transferred to quasi-Monte Carlo methods. The systematic study of importance sampling for quasi-Monte Carlo integration seems to have begun with the thesis of Chelson [4]. Later work, also on variants such as weighted uniform sampling and weighted importance sampling, includes Lambert [12], Maize [16], and Ökten [26]; see also Spanier and Maize [33, Section 4] for a survey of these methods. An analog of rejection sampling for quasi-Monte Carlo integration was considered by Wang [37]. Much remains to be done in this area, for instance, in the adaptation of other variance reduction techniques to quasi-Monte Carlo methods.

(ii) *Optimization of net constructions*. We use here the standard terminology in the theory of (t, m, s)-nets and (t, s)-sequences (see [13]; [20, Chapter 4]; [23, Chapter 8] for expository accounts of this theory). For fixed integers $m \geqslant 1$, $s \geqslant 1$, and $b \geqslant 2$, it is an important problem to determine the least value of t such that there exists a (t, m, s)-net in base b. A similar question can be asked for the restricted family of digital (t, m, s)-nets in base b. Except for obvious cases, very few answers are known. We have tables of lower and upper bounds for the least quality parameter t that can be achieved, for instance in [5,18], with recent partial updates in [29,31]. A new method of constructing digital nets, due to Niederreiter and Özbudak [22], is based on global function fields and has a great potential for setting many new records, at least for sufficiently large dimensions s and sufficiently large m.

Here is another optimization problem for nets: for fixed integers $t \geqslant 0$, $d \geqslant 2$, and $b \geqslant 2$, determine the largest dimension s for which there exists a (digital) $(t, t+d, s)$-net in base b. The study of an asymptotic version of this problem was initiated by Niederreiter and Xing [24]. Let q be a fixed prime power and $d \geqslant 2$ a given integer. Then it was shown in [24], as a consequence of a result of [32], that for any sequence of digital $(t_n, t_n + d, s_n)$-nets constructed over the finite field $\mathbb{F}_q$ with $s_n \to \infty$ as $n \to \infty$, we have

$$\liminf_{n \to \infty} \frac{t_n}{\log_q s_n} \geqslant \left\lfloor \frac{d}{2} \right\rfloor,$$

where $\log_q$ denotes the logarithm to the base q. It was also proved in [24] that if, in addition, a real number $\varepsilon > 0$ is given, then there exists a sequence of digital $(t_n, t_n + d, s_n)$-nets constructed over $\mathbb{F}_q$ such that $s_n \to \infty$ as $n \to \infty$ and

$$\lim_{n \to \infty} \frac{t_n}{\log_q s_n} \leqslant d + 1 + \varepsilon.$$

By a different construction, this was recently improved by Niederreiter and Xing [25] to

$$\lim_{n \to \infty} \frac{t_n}{\log_q s_n} \leqslant d - 1 - \left\lfloor \frac{d-1}{q} \right\rfloor.$$

Note that in view of the lower bound above, this result is best possible for $q = 2$. However, in most other cases there is still a gap between the lower and the upper bound.

If $t_b(s)$ denotes, as usual, the least value of t such that there exists a (t, s)-sequence in base b, then the order of magnitude of $t_b(s)$ as $s \to \infty$ is known, since we have

$$c_1(b)s \leqslant t_b(s) \leqslant c_2(b)s \quad \text{for } s \geqslant b + 1,$$

where $c_1(b)$ and $c_2(b)$ are positive constants depending only on b (see [23, Chapter 8]). The upper bound is obtained by a construction based on algebraic geometry. However, the exact determination of $t_b(s)$ is still open, except in a few relatively easy cases.

(iii) *Randomization and derandomization*. This topic is, in a sense, also connected with the topic of error reduction in (i). The idea of randomizing quasi-Monte Carlo methods for the purpose of error estimation is classical and goes back to Cranley–Patterson shifts for lattice rules. Expository accounts of randomized quasi-Monte Carlo methods can be found in the book of Fox [8, Chapter 14] and the survey article of L'Ecuyer and Lemieux [14].

Random shifts for arbitrary low-discrepancy sequences were considered by Tuffin [36]. A sophisticated scrambling scheme for nets was introduced and studied in detail by Owen (see [27] and the references in [28]). Many contributions to the analysis of this scrambling scheme are also due to Hickernell and his school (see the references in [39]). Loh [15] recently showed a central limit theorem for the quasi-Monte Carlo estimator afforded by scrambled $(0, m, s)$-nets. A simplified version of Owen's scrambling scheme was proposed by Matoušek [17].

For an s-dimensional digital net with generating matrices $C_1, \ldots, C_s$ over the finite field $\mathbb{F}_q$, scrambling can also be performed by premultiplying or postmultiplying $C_1, \ldots, C_s$ by a suitable nonsingular triangular matrix T over $\mathbb{F}_q$ (see [7]). If T is viewed as a random object, then this leads to a randomization of the given digital net. Tezuka [35] raised interesting questions on derandomizing such procedures. In particular, are there deterministic constructions for T which yield an improved performance of the scrambled digital net? Similar questions can be asked about shift parameters for low-discrepancy sequences and other randomization schemes.

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